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Conical diffraction by periodic structures: Variation of interfaces and gradient formulas

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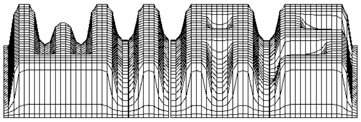

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This paper studies the dependence of solutions to conical diffraction problems upon geometric parameters of non–smooth profiles and interfaces between different materials of diffractive gratings. This problem arises in the design of those optical devices to diffract time–harmonic oblique incident plane waves to a specified far–field pattern. We prove the stability of solutions and give analytic formulas for the derivatives of reflection and transmission coefficients with respect to Lipschitz perturbations of interfaces. These derivatives are expressible as contour integrals involving the direct and adjoint solutions of conical diffraction problems.

1. Introduction

Diffractive optics is a modern technology in which optical devices are micromachined with complicated structural features on the order of the length of light waves. Exploiting diffraction effects, those devices can perform functions unattainable with conventional optics. Because of great advantages in terms of size and weight and many far–reaching applications in micro–optics, the optimal design of microoptical devices has received considerable attention in the engineering community and has stimulated several mathematical investigations.

One of the most common geometrical configurations is the so called periodic diffraction grating, which is formed by a periodic pattern of nonmagnetic materials (of permeability μ) with different dielectric constants ϵ. If the coordinate system is chosen such that the grating structure is periodic in the x_1–direction and invariant in the x_3–direction, then the diffraction problem is determined by the function $\epsilon(x_1, x_2)$ which is say d–periodic in x_1. This function is assumed to be piecewise constant and complex valued with $0 \leqslant \arg \epsilon < \pi$. Throughout, the material above and below the grating is assumed to be homogeneous with dielectric constants $\epsilon = \epsilon^+ > 0$ and ϵ^-, respectively. The grating is illuminated by an incoming plane electromagnetic wave

$$\mathbf{E}^i = \mathbf{p}\, e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3} e^{-i\omega t}\,, \quad \mathbf{H}^i = \mathbf{q}\, e^{i\alpha x_1 - i\beta x_2 + i\gamma x_3} e^{-i\omega t} \tag{1.1}$$

from the top with the angles of incidence $\theta, \phi \in (-\pi/2, \pi/2)$. In practical applications the wavelength $\lambda = 2\pi c/\omega$, c denoting the speed of light, is comparable to the period d. In this situation geometrical optics approximations to the underlying electromagnetic field equations are not accurate, hence, the mathematical modelling has to rely on Maxwell's equations or related partial differential equations.

The direct problem, i.e. the determination of the diffracted field for a given incident wave and some fixed periodic grating structure, is by now well understood. The case $\gamma = 0$ corresponds to the classical diffraction problem dating back to Rayleigh and Bloch. In that case Maxwell's equations reduce to the two scalar models of transverse electric (TE) and transverse magnetic (TM) polarization, and results on existence, uniqueness and regularity of solutions for rather general grating structures have been obtained during the last decade; see the references given in [9]. The underlying analysis is based on a variational approach which goes back to Achdou &Pironneau [1], Bonnet-Bendhia & Starling [2] and Bao & Dobson [5]. Recently [12] this approach was extended to the case $\gamma \neq 0$, the conical diffraction problem; see Section 2 for a review of some results.

A major part of the motivating applications in diffractive optics, however, is associated with the inverse problems of optimal interface shape design or profile reconstruction from scattered fields. To solve these problems via optimization methods, it is crucial to study the dependence of the diffracted field upon the grating structure, i.e. upon the piecewise constant coefficients of the underlying differential equations. Several recent articles are devoted to the regularity of the forward map which maps the dielectric coefficients to the solutions of the model. In particular, for the TE diffraction problem, rather general differentiability results as well as effective gradient formulas are known; see [1], [7], [3], [8]. The case of TM polarization, where the discontinuities occur in the principal part of the differential operator, is much more difficult to study than the TE case. In [3] it is shown that the forward map is Frechet differentiable with respect to variations of interfaces in the uniform norm, which however excludes the design of practically relevant diffractive structures. Existence of an optimal design for TM polarization is established in [4].

More precise regularity results for inverse TM diffraction problems can be obtained if the grating geometry is determined by a finite number of parameters. In [9] we derived explicit analytic formulas for the derivatives of cost functionals involving the reflection and transmission coefficients of binary diffractive gratings, where the derivatives have to be taken with respect to the transition points and the height of those gratings. Assuming that the solutions of the direct problem have only mild singularities at the corners of the grating profile, these derivatives can be expressed as one–dimensional integrals over the part of the interface to be varied. A new approach to this problem, which works for arbitrary singularities of the direct solution and also for more general non–smooth (e.g., polygonal) material interfaces, was given in [11].

In the present paper we extend these results to the diffraction of time–harmonic plane waves from periodic structures under oblique incidence. In Section 2 we briefly describe the conical diffraction problem including its variational formulation and review some basic results. In Section 3 we study the dependence of solutions to this problem with respect to rather general variations of the (non–smooth) grating profile and interfaces between different optical materials. Our result on the unique solvability of the perturbed problem is even new in the case of classical diffraction. In Section 4 we show that the derivatives of reflection and transmission coefficients can be represented as certain domain integrals. These formulas are simplified in Section 5 to get interface integrals or, in case of strong singularities of solutions, interface integrals plus point functionals. Alternative expressions in terms of path–independent contour integrals are derived in Section 6.

As in the classical diffraction case [10], the results may be used to develop gradient type optimization methods for solving design problems for diffraction by binary and multilevel gratings under oblique incidence. Further applications to the stability of the inverse problem of profile reconstruction from far field data will be given in a future publication.

2. Variational formulation

For notational convenience we will change the length scale by a factor of $2\pi/d$ so that the grating becomes 2π–periodic: $\epsilon(x_1 + 2\pi, x_2) = \epsilon(x_1, x_2)$. Note that this is equivalent to multiplying the frequency ω by $d/2\pi$. Then the wave vector of the incident field is expressed in terms of the angles of incidence as

$$\mathbf{k} = (\alpha, -\beta, \gamma) = k^+(\sin\theta\cos\phi, -\cos\theta\cos\phi, \sin\phi) \qquad \text{with } k^+ = \omega(\mu\epsilon^+)^{1/2} .$$

Note that $(\mathbf{E}^i, \mathbf{H}^i)$ satisfy the time–harmonic Maxwell equations if the constant amplitude vectors $\mathbf{p}$, $\mathbf{q}$ fulfil the relations $\mathbf{p} \cdot \mathbf{k} = 0$ and $\mathbf{q} = (\omega\mu)^{-1}\mathbf{k} \times \mathbf{p}$. Thus the incoming field is determined by two of their components, for example, p_3 and q_3.

Following [12] we transform Maxwell's equation to a simpler system of two–dimensional Helmholtz equations coupled via transmission conditions at the interfaces. The periodicity of ϵ, together with the form of the incident wave, motivates to seek for physical solutions $\mathbf{E}$ and $\mathbf{H}$ having the representation

$$(\mathbf{E},\mathbf{H})(x_1,x_2,x_3) = (\mathcal{E},\mathcal{H})(x_1,x_2)\,e^{i\gamma x_3}\,, \tag{2.1}$$

where $\mathcal{E},\mathcal{H}:\mathbb{R}^2\to\mathbb{C}^3$ are α quasi–periodic in x_1, i.e.

$$(\mathcal{E},\mathcal{H})(x_1+2\pi,x_2) = e^{2\pi i\alpha}(\mathcal{E},\mathcal{H})(x_1,x_2)\,.$$

Then the time–harmonic Maxwell equations for $(\mathbf{E},\mathbf{H})$ are equivalent to

$$(\partial_1,\partial_2,i\gamma)\times\mathcal{E} = i\omega\mu\mathcal{H}\ ,\ \ (\partial_1,\partial_2,i\gamma)\times\mathcal{H} = -i\omega\epsilon\mathcal{E} \tag{2.2}$$

in each subdomain in which ϵ is constant. The well–known jump conditions on the interface between two such subdomains take the form

$$[(\nu,0)\times\mathcal{E}]_{\Lambda\times\mathbb{R}} = [(\nu,0)\times\mathcal{H}]_{\Lambda\times\mathbb{R}} = 0 \tag{2.3}$$

where $(\nu,0) = (\nu_1,\nu_2,0)$ is the normal vector to the interface $\Lambda\times\mathbb{R}$ and $[(\nu,0)\times\mathcal{E}]_{\Lambda\times\mathbb{R}}$ denotes the jump of the function $(\nu,0)\times\mathcal{E}$ across the interface.

For the following we introduce the piecewise constant function

$$k = \sqrt{\omega^2\epsilon\mu}\,, \tag{2.4}$$

where the branch of the square-root is chosen such that $k>0$ for positive real arguments $\omega^2\epsilon\mu$ and its branch–cut is $(-\infty,0)$. Under the assumption that

$$k_\gamma^2 := k^2-\gamma^2 \neq 0\,, \tag{2.5}$$

it follows from (2.2) that

$$\begin{aligned}
\mathcal{E}_1 &= \frac{i}{k_\gamma^2}\,(\omega\mu\partial_2\mathcal{H}_3+\gamma\partial_1\mathcal{E}_3)\,, \qquad \mathcal{H}_1 = \frac{i}{k_\gamma^2}\,(-\omega\epsilon\partial_2\mathcal{E}_3+\gamma\partial_1\mathcal{H}_3)\,,\\
\mathcal{E}_2 &= \frac{i}{k_\gamma^2}\,(-\omega\mu\partial_1\mathcal{H}_3+\gamma\partial_2\mathcal{E}_3)\,, \quad \mathcal{H}_2 = \frac{i}{k_\gamma^2}\,(\omega\epsilon\partial_1\mathcal{E}_3+\gamma\partial_2\mathcal{H}_3)\,.
\end{aligned} \tag{2.6}$$

The third components $\mathcal{E}_3,\mathcal{H}_3$ satisfy Helmholtz equations

$$(\Delta+k_\gamma^2)\,\mathcal{E}_3 = (\Delta+k_\gamma^2)\,\mathcal{H}_3 = 0 \tag{2.7}$$

in each of the domains in which ϵ is constant, and the jump conditions are transformed to the transmission conditions

$$[\mathcal{E}_3]_\Lambda = [\mathcal{H}_3]_\Lambda = 0\,,\ \left[\frac{\gamma}{k_\gamma^2}\partial_\tau\mathcal{H}_3+\frac{\omega\epsilon}{k_\gamma^2}\partial_\nu\mathcal{E}_3\right]_\Lambda = \left[\frac{\gamma}{k_\gamma^2}\partial_\tau\mathcal{E}_3-\frac{\omega\mu}{k_\gamma^2}\partial_\nu\mathcal{H}_3\right]_\Lambda = 0\,, \tag{2.8}$$

at the interfaces Λ, where $\partial_\tau = \nu_1\partial_2-\nu_2\partial_1$ is the tangential derivative and $[\cdot]_\Lambda$ denotes the jump across the interface Λ.

Due to the quasi–periodicity of $\mathcal{E}_3, \mathcal{H}_3$ we consider the problem in the strip $x_1 \in (0, 2\pi)$, and define the functions $u = e^{-i\alpha x_1}\,\mathcal{E}_3$, $v = e^{-i\alpha x_1}\,\mathcal{H}_3$, which are 2π–periodic in x_1. Defining the operators

$$\nabla_\alpha = \nabla + i\,(\alpha, 0)\ ,\ \Delta_\alpha = \nabla_\alpha \cdot \nabla_\alpha = \Delta + 2i\alpha\partial_1 - \alpha^2\ ,$$
$$\partial_{\nu,\alpha} = \nu \cdot \nabla_\alpha\ ,\ \partial_{\tau,\alpha} = \nu_1\partial_2 - \nu_2\partial_1 - i\alpha\nu_2\ ,$$

(2.7) and (2.8) are transformed to the differential equations

$$(\Delta_\alpha + k_\gamma^2)\,u = (\Delta_\alpha + k_\gamma^2)\,v = 0 \quad \text{in } \mathbb{R}^2 \tag{2.9}$$

and the transmission conditions

$$\begin{gathered}[u]_\Lambda = [v]_\Lambda = 0\\ \left[\frac{\gamma}{k_\gamma^2}\partial_{\tau,\alpha}u - \frac{\omega\mu}{k_\gamma^2}\partial_{\nu,\alpha}v\right]_{\Lambda_j} = \left[\frac{\gamma}{k_\gamma^2}\partial_{\tau,\alpha}v + \frac{\omega\epsilon}{k_\gamma^2}\partial_{\nu,\alpha}u\right]_\Lambda = 0\,,\end{gathered} \tag{2.10}$$

which have to be satisfied together with periodic boundary conditions. Because the domain is unbounded in the x_2–direction, a radiation condition must be imposed ensuring the finite energy of the scattered field. Since the factors $\mathcal{E}, \mathcal{H}$ in (2.1) are analytic and α–quasiperiodic above and below the grating, this condition implies that they admit a representation as a sum of outgoing bounded plane waves plus the incoming plane wave.

Applied to the functions u and v this means the following: If we choose $b \in \mathbb{R}$ such that the material remains homogeneous for $|x_2| \geqslant b$, i.e. $\epsilon(x_1, \pm x_2) = \epsilon^\pm$, $x_2 \geqslant b$, then the representations

$$\begin{aligned} u(x_1,x_2) &= \sum_{n\in\mathbb{Z}} E_n^+ e^{inx_1 + i\beta_n^+ x_2} + p_3 e^{-i\beta x_2}\ ,\\ v(x_1,x_2) &= \sum_{n\in\mathbb{Z}} H_n^+ e^{inx_1 + i\beta_n^+ x_2} + q_3 e^{-i\beta x_2}\ ,\\ u(x_1,x_2) &= \sum_{n\in\mathbb{Z}} E_n^- e^{inx_1 - i\beta_n^- x_2}\ ,\quad v(x_1,x_2) = \sum_{n\in\mathbb{Z}} H_n^- e^{inx_1 - i\beta_n^- x_2}\ ,\end{aligned} \tag{2.11}$$

are valid with unknown complex constants $E_n^\pm, H_n^\pm$. Here we use the notation

$$\beta_n^\pm = \beta_n^\pm(\alpha) = \sqrt{(k^\pm)^2 - \gamma^2 - (n+\alpha)^2}\,,\ n \in \mathbb{Z}\,, \tag{2.12}$$

where the square-root is defined as in equation (2.4). The so–called Rayleigh amplitudes $E_n^\pm, H_n^\pm$ define the diffraction pattern of the grating and their exact computation is the final goal of direct diffraction problems. More details can be found in [14, 12].

Now the problem can be reduced to the rectangular cell $\Omega = (0, 2\pi) \times (-b, b)$. Let us denote by $H_p^s(\Omega)$, $s \geqslant 0$, the restriction to Ω of all functions in the Sobolev space $H_{loc}^s(\mathbb{R}^2)$ which are 2π–periodic in x_1. Note that if $f, g \in H_p^1(\Omega)$ and $\Omega_0 \subset \Omega$ has Lipschitz boundary, then Green's formula yields the identities

$$\int_{\Omega_0} \Delta_\alpha f\,\overline{g} = -\int_{\Omega_0} \nabla_\alpha f\,\overline{\nabla_\alpha g} + \int_{\partial\Omega_0} \partial_{\nu,\alpha} f\,\overline{g}\ ,\quad \int_{\Omega_0} \nabla_\alpha g\,\overline{\nabla_\alpha^\perp f} = -\int_{\partial\Omega_0} \partial_{\tau,\alpha} g\,\overline{f}\ , \tag{2.13}$$

where we use the notation $\nabla_\alpha^\perp := (\partial_2, -\partial_1) - i\,(0, \alpha)$.

Let Ω_j, $j=1,\dots,m$, be the subdomains of Ω in which ϵ does not jump. Throughout the paper the boundaries $\partial\Omega_j$ are supposed to be piecewise smooth having corners with angles strictly between 0 and 2π. In the following the set $(\cup_j \partial\Omega_j)\setminus\partial\Omega$ of all interface points lying in the bounded cell Ω will be denoted by Λ. It contains only a finite number of singular points where smooth arcs meet at a corner or may intersect each other.

To obtain the variational form of the conical diffraction problem, we multiply the equations (2.9) in each subdomain Ω_j by the constant factors $\omega\epsilon/k_\gamma^2$ and $\omega\mu/k_\gamma^2$, respectively. The application of the first identity in (2.13) with $\varphi,\psi\in H_p^1(\Omega)$ leads to the equations

$$\begin{aligned}
&\sum_{j=1}^{m}\Big(\int_{\Omega_j}\Big(\frac{\omega\epsilon}{k_\gamma^2}\nabla_\alpha u\,\overline{\nabla_\alpha\varphi}-\omega\epsilon\,u\,\overline{\varphi}\Big)-\int_{\partial\Omega_j}\frac{\omega\epsilon}{k_\gamma^2}\,\partial_{\nu,\alpha}u\,\overline{\varphi}\Big)=0\,,\\
&\sum_{j=1}^{m}\Big(\int_{\Omega_j}\Big(\frac{\omega\mu}{k_\gamma^2}\,\nabla_\alpha v\,\overline{\nabla_\alpha\psi}-\omega\mu\,v\,\overline{\psi}\Big)-\int_{\partial\Omega_j}\frac{\omega\mu}{k_\gamma^2}\,\partial_{\nu,\alpha}v\,\overline{\psi}\Big)=0\,.
\end{aligned}\tag{2.14}$$

Using the second identity in (2.13) and the transmission condition on the interface Λ, we obtain the equivalent equations

$$\begin{aligned}
&\sum_j\int_{\Omega_j}\Big(\frac{\omega\epsilon}{k_\gamma^2}\nabla_\alpha u\overline{\nabla_\alpha\varphi}-\frac{\gamma}{k_\gamma^2}\nabla_\alpha v\overline{\nabla_\alpha^\perp\varphi}-\omega\epsilon u\overline{\varphi}\Big)-\int_{\partial\Omega}\Big(\frac{\omega\epsilon}{k_\gamma^2}\partial_{\nu,\alpha}u+\frac{\gamma}{k_\gamma^2}\partial_{\tau,\alpha}v\Big)\,\overline{\varphi}=0\,,\\
&\sum_j\int_{\Omega_j}\Big(\frac{\omega\mu}{k_\gamma^2}\nabla_\alpha v\,\overline{\nabla_\alpha\psi}+\frac{\gamma}{k_\gamma^2}\nabla_\alpha u\overline{\nabla_\alpha^\perp\psi}-\omega\mu v\overline{\psi}\Big)-\int_{\partial\Omega}\Big(\frac{\omega\mu}{k_\gamma^2}\partial_{\nu,\alpha}v-\frac{\gamma}{k_\gamma^2}\partial_{\tau,\alpha}u\Big)\,\overline{\psi}=0\,,
\end{aligned}\tag{2.15}$$

which must hold for all $\varphi,\psi\in H_p^1(\Omega)$.

Since all functions are periodic in x_1, the boundary integrals in (2.15) consist of integrals over the artificial boundaries $\Gamma^\pm=\{(x_1,\pm b),x_1\in[0,2\pi]\}$. If we introduce the matrix functions

$$M_n^\pm=\frac{1}{(k^\pm)^2-\gamma^2}\begin{pmatrix}-i\omega\epsilon\beta_n^\pm & \pm i\gamma(n+\alpha)\\ \mp i\gamma(n+\alpha) & -i\omega\mu\beta_n^\pm\end{pmatrix}\,,\tag{2.16}$$

then the boundary operators applied to functions u and v satisfying (2.11) can be represented in the form

$$\begin{aligned}
&\begin{pmatrix}(\omega\epsilon\partial_{\nu,\alpha}u+\gamma\partial_{\tau,\alpha}v)/k_\gamma^2\\ (\omega\mu\partial_{\nu,\alpha}v-\gamma\partial_{\tau,\alpha}u)/k_\gamma^2\end{pmatrix}\Bigg|_{\Gamma^+}=-\sum_{n\in\mathbb{Z}}M_n^+\begin{pmatrix}E_n^+\\ H_n^+\end{pmatrix}e^{inx_1+i\beta_n^+b}-\frac{i\omega\beta\,e^{-i\beta b}}{(k^+)^2-\gamma^2}\begin{pmatrix}\epsilon\,p_3\\ \mu\,q_3\end{pmatrix},\\
&\begin{pmatrix}(\omega\epsilon\partial_{\nu,\alpha}u+\gamma\partial_{\tau,\alpha}v)/k_\gamma^2\\ (\omega\mu\partial_{\nu,\alpha}v-\gamma\partial_{\tau,\alpha}u)/k_\gamma^2\end{pmatrix}\Bigg|_{\Gamma^-}=-\sum_{n\in\mathbb{Z}}M_n^-\begin{pmatrix}E_n^-\\ H_n^-\end{pmatrix}e^{inx_1+i\beta_n^-b}\,.
\end{aligned}\tag{2.17}$$

On the other hand, defining the operators $T_\alpha^\pm$ acting on 2π-periodic vector functions on $\mathbb{R}$

$$(T_\alpha^\pm w)(x)=\sum_{n\in\mathbb{Z}}M_n^\pm\hat{w}_n e^{inx}\,,\quad \hat{w}_n=(2\pi)^{-1}\int_0^{2\pi}w(x)\,e^{-inx}\,dx\,,\tag{2.18}$$

then for functions u and v satisfying (2.11)

$$\begin{aligned}
T_\alpha^+\begin{pmatrix}u\\ v\end{pmatrix}&=\sum_{n\in\mathbb{Z}}M_n^+\begin{pmatrix}E_n^+\\ H_n^+\end{pmatrix}e^{inx_1+i\beta_n^+b}-\frac{i\omega\beta\,e^{-i\beta b}}{(k^+)^2-\gamma^2}\begin{pmatrix}\epsilon\,p_3\\ \mu\,q_3\end{pmatrix}\,,\\
T_\alpha^-\begin{pmatrix}u\\ v\end{pmatrix}&=\sum_{n\in\mathbb{Z}}M_n^-\begin{pmatrix}E_n^-\\ H_n^-\end{pmatrix}e^{inx_1+i\beta_n^-b}\,,
\end{aligned}\tag{2.19}$$

where $T_\alpha^\pm(u,v)$ denote the action of these pseudodifferential operators on the traces $(u,v)|_{\Gamma^\pm} \in (H_p^{s-1/2}(\Gamma^\pm))^2$.

Therefore, combining (2.15), (2.17) and (2.19), the conical diffraction problem (2.9) – (2.11) can now be formulated as follows: Find $u, v \in H_p^1(\Omega)$ such that

$$\begin{aligned}\mathcal{B}\Big(\binom{u}{v},\binom{\varphi}{\psi}\Big) &:= B_\epsilon(u,\varphi) + B_\mu(v,\psi) - C(v,\varphi) + C(u,\psi)\\ &\quad + \int\limits_{\Gamma^+} T_\alpha^+\binom{u}{v}\cdot\binom{\overline{\varphi}}{\overline{\psi}} + \int\limits_{\Gamma^-} T_\alpha^-\binom{u}{v}\cdot\binom{\overline{\varphi}}{\overline{\psi}}\\ &= -\frac{2i\,e^{-i\beta b}}{k_\gamma^2}\int\limits_{\Gamma^+}\Big(\omega\epsilon^+ p_3\,\overline{\varphi} + \omega\mu q_3\,\overline{\psi}\Big), \quad \forall \varphi,\psi \in H_p^1(\Omega)\,,\end{aligned} \tag{2.20}$$

where we denote

$$B_\sigma(u,\varphi) = \int\limits_{\Omega}\Big(\frac{\omega\sigma}{k_\gamma^2}\nabla_\alpha u\,\overline{\nabla_\alpha\varphi} - \omega\sigma\,u\overline{\varphi}\Big)\,, \quad C(v,\varphi) = \int\limits_{\Omega}\frac{\gamma}{k_\gamma^2}\nabla_\alpha v\,\overline{\nabla_\alpha^\perp\varphi}\,. \tag{2.21}$$

Under the assumption on the dielectric coefficients ϵ of the materials and the incidence angle ϕ that

$$0 \leqslant \arg\epsilon < \pi\ ,\ \epsilon^+ > 0\ , \quad \text{and} \quad \epsilon > \epsilon^+\sin^2\phi \quad \text{for real } \epsilon, \tag{2.22}$$

it was proved in [12] that the sesquilinear form $\mathcal{B}$ is strongly elliptic in the following sense: The form

$$\mathcal{A}\Big(\binom{u}{v},\binom{\varphi}{\psi}\Big) := \mathcal{B}\Big(\binom{u}{v},\binom{\varphi}{\psi}\Big) + \int\limits_{\Omega}(\omega\epsilon\,u\overline{\varphi} + \omega\mu\,v\overline{\psi}) \tag{2.23}$$

is coercive after multiplying by some complex number ρ:

$$\operatorname{Re}\rho\mathcal{A}\Big(\binom{u}{v},\binom{u}{v}\Big) \geqslant c\,\omega\,\Big\|\binom{u}{v}\Big\|_{H_p^1(\Omega)}.$$

Moreover, the constant c depends only on the incidence angles $\theta, \phi \in (-\pi/2, \pi/2)$, and the graph of the piecewise constant function ϵ. The following existence and regularity results hold (cf .[12]):

1. If $\mathrm{Im}\ \epsilon > 0$ in some subdomain $\Omega_1 \subset \Omega$ then the variational problem (2.20) has a unique solution $(u,v) \in (H_p^1(\Omega))^2$ for all $\omega > 0$.

2. Assume that $\epsilon^- > \epsilon^+(1-\cos^2\theta\cos^2\phi)$ if ϵ^- is real.
   (i) The diffraction problem (2.20) is solvable in $(H_p^1(\Omega))^2$ for any frequency ω.
   (ii) For all but a countable set of frequencies ω_j, $\omega_j \to \infty$, one has unique solvability.

3. If for $(\omega^0, \theta^0, \phi^0) \notin \mathcal{R}$ the equation (2.20) is uniquely solvable, then the solution depends analytically on ω, θ, ϕ in a neighbourhood of this point. Here $\mathcal{R}$ is the set of Rayleigh frequencies

$$\mathcal{R} = \Big\{(\omega,\theta,\phi) : \exists\, n \in \mathbb{Z}\ \text{ s. th. }\ \omega^2\mu(\epsilon^\pm - \epsilon^+\sin^2\phi) = (n + \omega^2\mu\epsilon^+\sin^2\theta\cos^2\phi)\Big\}$$

Note that for $\gamma = 0$ the form $\mathcal{C}$ vanishes, the factor $\omega\epsilon/k_\gamma^2$ becomes constant in Ω and the system (2.20) decouples into scalar problems for u and v corresponding to the TE and TM polarisation, respectively.

3. Variation of interfaces

We are interested in the solvability of the conical diffraction problem and the dependence of Rayleigh amplitudes $E_n^\pm$ and $H_n^\pm$ if parts of the interfaces Λ between different materials are varied to some new interfaces Λ_h. This variation leads to a new piecewise constant function $k_h^2 = \omega^2 \epsilon_h \mu$ and to the corresponding diffraction problem

$$\mathcal{B}^h\Big(\binom{u}{v},\binom{\varphi}{\psi}\Big) = -\frac{2i\, e^{-i\beta b}}{k_\gamma^2} \int\limits_{\Gamma^+} \Big(\omega\epsilon^+ p_3\, \overline{\varphi} + \omega\mu q_3\, \overline{\psi}\Big), \quad \forall \varphi, \psi \in H_p^1(\Omega)\,, \tag{3.1}$$

representing a strong perturbation of the original problem. However, the unique solvability is retained under the mild assumption that the operator of multiplication by $\epsilon_h - \epsilon$ converges strongly to zero in $L^2(\Omega)$,

$$\|(\epsilon_h - \epsilon)u\|_{L^2(\Omega)} \to 0 \text{ as } h \to 0\,, \quad \forall\, u \in L^2(\Omega)\,. \tag{3.2}$$

Theorem 3.1 If for fixed parameters ω, θ and ϕ the conical diffraction problem (2.20) has a unique solution (u, v) and the perturbation of the grating satisfies (3.2), then for all sufficiently small h the perturbed problems (3.1) are also uniquely solvable. Their solutions converge to (u, v) in the norm of H^1.

Proof. One can use standard arguments from the theory of projection methods. The forms $\mathcal{B}^h(\cdot,\cdot)$ generate a sequence of bounded operators, denoted again by $\mathcal{B}^h$ and acting from $(H_p^1(\Omega))^2$ into its dual $((H_p^1(\Omega))^2)'$, which in view of (3.2) converge strongly to $\mathcal{B}$. Suppose that there exists a sequence $U_h = (u_h, v_h) \in (H_p^1(\Omega))^2$, $\|U_h\| = 1$, such that $\mathcal{B}^h U_h \to 0$. A subsequence, again denoted by $\{U_h\}$, converges weakly to some $U \in (H_p^1(\Omega))^2$, hence $U = 0$. On the other hand, as mentioned above, the operators allow the representation $\mathcal{B}^h = \mathcal{A}^h + \mathcal{T}^h$, where

$$\rho(\mathcal{A}^h U_h, U_h) \geqslant c\,\omega\, \|U_h\|_{(H_p^1(\Omega))^2}$$

with a constant c depending only on the graph of ϵ_h, i.e. not depending on h. Furthermore,

$$\mathcal{T}^h U_h = -\omega(\epsilon_h u_h + \mu v_h) \to 0\,,$$

contradicting the assumption $\|U_h\| = 1$. ∎

To study the convergence of the solutions U_h of the perturbed problems (3.1) to the solution U of the original problem, we consider a more regular perturbation of the interfaces assuming that, for sufficiently small $|h|$, the perturbed interface Λ_h is given by

$$\Lambda_h = \Phi_h(\Lambda)\,, \ \Phi_h(x) = x + h\,\chi(x)\,. \tag{3.3}$$

Here Φ_h is a Lipschitz diffeomorphism of Ω onto itself, and $\chi = (\chi_1, \chi_2)$ is 2π–periodic in x_1 and has compact support in $[0, 2\pi] \times (-b, b)$.

Then we can define the isomorphism $\Psi_h : H_p^1(\Omega) \to H_p^1(\Omega)$ which maps u to $u \circ \Phi_h^{-1}$. Moreover, $\epsilon_h = \Psi_h \epsilon$, $k_h = \Psi_h k$ and the change of variables $y = \Phi_h(x)$ provides

$$dy = |J(x)|dx$$

with

$$J(x) = 1 + h\Big(\frac{\partial\chi_1}{\partial x_1} + \frac{\partial\chi_2}{\partial x_2}\Big) + h^2\Big(\frac{\partial\chi_1}{\partial x_1}\frac{\partial\chi_2}{\partial x_2} - \frac{\partial\chi_1}{\partial x_2}\frac{\partial\chi_2}{\partial x_1}\Big)$$

and

$$\frac{\partial}{\partial y_1} = \frac{1 + h\,\partial\chi_2/\partial x_2}{J(x)}\frac{\partial}{\partial x_1} - \frac{h\,\partial\chi_2/\partial x_1}{J(x)}\frac{\partial}{\partial x_2}\,,$$
$$\frac{\partial}{\partial y_2} = -\frac{h\,\partial\chi_1/\partial x_2}{J(x)}\frac{\partial}{\partial x_1} + \frac{1 + h\,\partial\chi_1/\partial x_1}{J(x)}\frac{\partial}{\partial x_2}\,.$$

Hence we obtain

$$\begin{aligned}
B^h_\epsilon(\Psi_h u, \Psi_h\varphi) &= \int\limits_\Omega \Big(\frac{\omega\epsilon_h(y)}{k_h^2(y) - \gamma^2}\nabla_\alpha\Psi_h u \cdot \overline{\nabla_\alpha\Psi_h\varphi} - \omega\epsilon_h(y)\Psi_h u\overline{\Psi_h\varphi}\Big)\,dy \\
&= \int\limits_\Omega \frac{\omega\epsilon((1 + h\partial_2\chi_2)\partial_1 + i\alpha J(x) - h\partial_1\chi_2\partial_2)u\,((1 + h\partial_2\chi_2)\partial_1 - i\alpha J(x) - h\partial_1\chi_2\partial_2)\overline{\varphi}}{J(x)k_\gamma^2(x)}\,dx \\
&+ \int\limits_\Omega \frac{\omega\epsilon(- h\partial_2\chi_1\partial_1 + (1 + h\partial_1\chi_1)\partial_2)u\,(- h\partial_2\chi_1\partial_1 + (1 + h\partial_1\chi_1)\partial_2)\overline{\varphi}}{J(x)k_\gamma^2(x)}\,dx \\
&- \int\limits_\Omega \omega\epsilon u\,\overline{\varphi}\,J(x)\,dx = B_\epsilon(u,\varphi) + hB_{\epsilon,1}(u,\varphi) + h^2B^h_{\epsilon,2}(u,\varphi)\,,
\end{aligned} \tag{3.4}$$

where

$$\begin{aligned}
B_{\epsilon,1}(u,\varphi) &= -\int\limits_\Omega \omega\epsilon(\partial_1\chi_1 + \partial_2\chi_2)u\,\overline{\varphi}\Big) \\
&- \int\limits_\Omega \frac{\omega\epsilon}{k_\gamma^2}\Big(\partial_1\chi_2(\partial_{1,\alpha}u\,\overline{\partial_2\varphi} + \partial_2 u\,\overline{\partial_{1,\alpha}\varphi}) + \partial_2\chi_1(\partial_1 u\,\overline{\partial_2\varphi} + \partial_2 u\,\overline{\partial_1\varphi}\Big) \\
&+ \int\limits_\Omega \frac{\omega\epsilon}{k_\gamma^2}\Big(\partial_2\chi_2(\partial_{1,\alpha}u\,\overline{\partial_{1,\alpha}\varphi} - \partial_2 u\,\overline{\partial_2\varphi}) + \partial_1\chi_1(\partial_2 u\,\overline{\partial_2\varphi} - \partial_1 u\,\overline{\partial_1\varphi} + \alpha^2 u\,\overline{\varphi})\Big)
\end{aligned} \tag{3.5}$$

and the remainder term satisfies

$$|B^h_{\epsilon,2}(u,\varphi)| \leqslant c\|u\|_1\|\varphi\|_1\ ,\ u,\varphi \in H^1_p(\Omega\ ,\ |h| \leqslant h_0\,.$$

Here we have used the notation $\partial_j = \partial/\partial x_j$, $\partial_{1,\alpha} = \partial_1 + i\alpha$ and the relation

$$J(x)^{-1} = 1 - h(\partial_1\chi_1 + \partial_2\chi_2) + O(h^2)\,,\ |h| \leqslant h_0\,,$$

which holds uniformly in $x \in \Omega$.

Since μ is constant in Ω, the form $B^h_\mu(\Psi_h u, \Psi_h\varphi)$ admits an expansion with ϵ replaced by μ in (3.4). The off–diagonal form has the expansion

$$\begin{aligned}
C^h(\Psi_h v, \Psi_h\varphi) &= \int\limits_\Omega \frac{\gamma}{k_h^2(y) - \gamma^2}\nabla_\alpha\Psi_h v\overline{\nabla_\alpha^\perp\Psi_h\varphi}\,dy \\
&= \int\limits_\Omega \frac{\gamma((1 + h\partial_2\chi_2)\partial_1 + i\alpha J(x) - h\partial_1\chi_2\partial_2)v\,(- h\partial_2\chi_1\partial_1 + (1 + h\partial_1\chi_1)\partial_2)\overline{\varphi}}{J(x)k_\gamma^2(x)}\,dx \\
&- \int\limits_\Omega \frac{\gamma(- h\partial_2\chi_1\partial_1 + (1 + h\partial_1\chi_1)\partial_2)v\,((1 + h\partial_2\chi_2)\partial_1 - i\alpha J(x) - h\partial_1\chi_2\partial_2)\overline{\varphi}}{J(x)k_\gamma^2(x)}\,dx \\
&= C(v,\varphi) + hC_1(v,\varphi) + h^2C^h_2(v,\varphi)\,,
\end{aligned}$$

where

$$C_1(v,\varphi) \;=\sum_j \int\limits_{\Omega_j} \frac{i\alpha\gamma}{k_\gamma^2}(\partial_1\chi_1(v\overline{\partial_2\varphi}+\partial_2 v\overline{\varphi})-\partial_2\chi_1(v\overline{\partial_1\varphi}+\partial_1 v\overline{\varphi})) \tag{3.6}$$

and the remainder term satisfies

$$|C_2^h(v,\varphi)| \leqslant c\|v\|_1\|\varphi\|_1\,,\; v,\varphi\in H_p^1(\Omega\,,\;|h|\leqslant h_0\,.$$

Since the substitution $y=\Phi_h(x)$ in the sesquilinear form $\mathcal{B}^h$ does not change the boundary terms, we have for $|h|\leqslant h_0$

$$\begin{aligned}&\mathcal{B}^h\left(\binom{\Psi_h u}{\Psi_h v},\binom{\Psi_h\varphi}{\Psi_h\psi}\right)\\ &=\mathcal{B}\left(\binom{u}{v},\binom{\varphi}{\psi}\right)+h\left(B_{\epsilon,1}(u,\varphi)+B_{\mu,1}(v,\psi)-C_1(v,\varphi)+C_1(u,\psi)\right)\\ &\quad+h^2\left(B_{\epsilon,2}^h(u,\varphi)+B_{\mu,2}^h(v,\psi)-C_2^h(v,\varphi)+C_2^h(u,\psi)\right).\end{aligned} \tag{3.7}$$

THEOREM 3.2 If the perturbation of the grating geometry is given by the regular mapping (3.3), then the solution of this problem takes the form

$$\Psi_h^{-1}u_h=u+hu_1+h^2u_{2,h}\,,\quad \Psi_h^{-1}v_h=v+hv_1+h^2v_{2,h}\,, \tag{3.8}$$

where (u,v) is the solution of the original problem (2.20), $(u_1,v_1)\in(H_p^1(\Omega))^2$ solves the equation

$$\mathcal{B}\left(\binom{u_1}{v_1},\binom{\varphi}{\psi}\right)=-B_{\epsilon,1}(u,\varphi)-B_{\mu,1}(v,\psi)+C_1(v,\varphi)-C_1(u,\psi)\,,\;\forall\,\varphi,\psi\in H_p^1(\Omega), \tag{3.9}$$

and the remainders satisfy $\|u_{2,h}\|_1,\|v_{2,h}\|_1\leqslant c$ for $|h|\leqslant h_0$.

Proof. Inserting the ansatz (3.8) for the solution U_h of (3.1) into (3.7), yields equation (3.9) for (u_1,v_1). For $(u_{2,h},v_{2,h})$ one gets a similar equation with uniformly bounded right–hand side. ∎

REMARK 3.1 One can prove recursively that for any $N\geqslant 2$ the solution of (3.1) admits the expansion

$$\Psi_h^{-1}u_h=\sum_{j=0}^N h^j u_j+h^{N+1}u_{N+1,h}\,,\quad \Psi_h^{-1}v_h=\sum_{j=0}^N h^j v_j+h^{N+1}v_{N+1,h}\,,$$

with $u_0:=u,u_1,v_0:=v,v_1$ as above, certain functions $u_j,v_j\in H_p^1(\Omega)$, $j\geqslant 2$, and remainders satisfying $\|u_{N+1,h}\|_1,\|v_{N+1,h}\|_1\leqslant c_N$.

4. Optimization of grating efficiencies

Define the finite sets of indices $P^\pm=\{n\in\mathbb{Z}:\beta_n^\pm>0\}$, where $\beta_n^\pm$ is given by (2.12). Then the Rayleigh amplitudes $E_n^\pm$ and $H_n^\pm$, $n\in P^\pm$, correspond to the propagating modes of the fields $\mathcal{E}, \mathcal{H}$ and can be obtained from the traces of the solution u, v of the problem (2.20) on the artificial boundaries $\Gamma^{\pm}$,

$$\left.\begin{aligned} E_n^+ &= -p_3\,\delta_{0n} e^{-2i\beta b} + \frac{e^{-i\beta_n^+ b}}{2\pi} \int\limits_{\Gamma^+} u\, e^{-inx_1}\, dx_1\,, \\ H_n^+ &= -q_3\,\delta_{0n} e^{-2i\beta b} + \frac{e^{-i\beta_n^+ b}}{2\pi} \int\limits_{\Gamma^+} v\, e^{-inx_1}\, dx_1\,, \end{aligned}\right\} \qquad n \in P^+\,,$$
$$E_n^- = \frac{e^{-i\beta_n^- b}}{2\pi} \int\limits_{\Gamma^-} u\, e^{-inx_1}\, dx_1\,,\ H_n^- = \frac{e^{-i\beta_n^- b}}{2\pi} \int\limits_{\Gamma^-} v\, e^{-inx_1}\, dx_1\,, \quad n \in P^-\,. \tag{4.1}$$

These reflection and transmission coefficients are used to compute the so called conical diffraction efficiencies of the grating, which are defined by

$$e_n^+ = \frac{\beta_n^+}{\beta} \frac{\epsilon^+|E_n^+|^2 + \mu|H_n^+|^2}{\epsilon^+|p_3|^2 + \mu|q_3|^2}\,,\ e_n^- = \frac{k_+^2 - \gamma^2}{k_-^2 - \gamma^2} \frac{\beta_n^+}{\beta} \frac{\epsilon^-|E_n^-|^2 + \mu|H_n^-|^2}{\epsilon^+|p_3|^2 + \mu|q_3|^2}\,.$$

If the energy of the incoming field is normalized to $\epsilon^+|p_3|^2 + \mu|q_3|^2 = 1$, then the efficiencies $e_n^{\pm}$ represent the energy of the reflected or transmitted plane waves of order $n \in P^{\pm}$ with the corresponding wave vector $(\alpha_n, \pm\beta_n^{\pm}, \gamma)$. For dielectric gratings, i.e. the dielectric coefficients ϵ of all materials are real, the principle of conservation of energy then yields the relation

$$\sum_{n \in P^+} e_n^+ + \sum_{n \in P^-} e_n^- = 1\,, \tag{4.2}$$

whereas for metallic gratings the total sum of the efficiencies is less than 1. Note that $P^- = \emptyset$ if $\mathrm{Im}\ \epsilon^- \neq 0$.

The problem of designing a diffractive grating, which gives rise to a specified far–field pattern, can often be viewed as a minimization problem for some function F depending smoothly on the Rayleigh amplitudes:

$$F = F(E_n^+, H_n^+, E_n^-, H_n^-)\,.$$

To find local minima of F, gradient–type or higher order optimization algorithms are advantageous. It can be easily seen that for fixed parameters ω, θ and ϕ the function F is differentiable with respect to regular perturbations (3.3) of the interface Λ. Indeed, since $\Psi_h \varphi|_{\Gamma^{\pm}} = \varphi|_{\Gamma^{\pm}}$ for any $\varphi \in H_p^1(\Omega)$, it follows from Theorem 3.2 that the derivatives of $E_n^{\pm}, H_n^{\pm}$ with respect to the Lipschitz diffeomorphism $\Phi_h(x) = x + h\,\chi(x)$ are given by

$$\begin{aligned} DE_n^{\pm}(\chi) &= \lim_{h \to 0} \frac{e^{-i\beta_n^{\pm} b}}{2\pi h} \int\limits_{\Gamma^{\pm}} (u_h - u)\, e^{-inx_1}\, dx_1 = \frac{e^{-i\beta_n^{\pm} b}}{2\pi} \int\limits_{\Gamma^{\pm}} u_1\, e^{-inx_1}\, dx_1\,, \\ DH_n^{\pm}(\chi) &= \lim_{h \to 0} \frac{e^{-i\beta_n^{\pm} b}}{2\pi h} \int\limits_{\Gamma^{\pm}} (v_h - v)\, e^{-inx_1}\, dx_1 = \frac{e^{-i\beta_n^{\pm} b}}{2\pi} \int\limits_{\Gamma^{\pm}} v_1\, e^{-inx_1}\, dx_1\,, \end{aligned} \tag{4.3}$$

where (u_h, v_h) is the solution of the diffraction problem (3.1) with the perturbed geometry (3.3) and (u_1, v_1) solves (3.9). Hence the derivative of F is given by

$$DF(\chi) = \sum a_n^{\pm} DE_n^{\pm}(\chi) + \sum b_n^{\pm} DH_n^{\pm}(\chi)\,.$$

with known coefficients $a_n^\pm$ and $b_n^\pm$ (depending in general on $E_n^\pm$ and $H_n^\pm$).

Now let (w,z) denote the solution of the adjoint problem

$$\mathcal{B}\left(\binom{\varphi}{\psi},\binom{w}{z}\right) = \sum a_n^\pm \frac{e^{-i\beta_n^\pm b}}{2\pi} \int\limits_{\Gamma^\pm} \varphi\, e^{-inx_1} + \sum b_n^\pm \frac{e^{-i\beta_n^\pm b}}{2\pi} \int\limits_{\Gamma^\pm} \psi\, e^{-inx_1}\,, \tag{4.4}$$

for all $\varphi,\psi \in H_p^1(\Omega)$. Taking $\varphi = 0, \psi = 0$ on $\Gamma^\pm$ and using (2.13), one obtains

$$\begin{aligned}\mathcal{B}\left(\binom{\varphi}{\psi},\binom{w}{z}\right) &= -\int\limits_{\Omega} \left(\varphi\left(\nabla_\alpha \frac{\omega\epsilon}{k_\gamma^2}\nabla_\alpha\overline{w} - \omega\epsilon\overline{w}\right) + \psi\left(\nabla_\alpha \frac{\omega\mu}{k_\gamma^2}\nabla_\alpha\overline{z} - \omega\mu\overline{z}\right)\right)\\ &+ \sum_j \int\limits_{\Omega_j} \left(\varphi\frac{\omega\epsilon}{k_\gamma^2}\overline{\partial_{\nu,\alpha} w} + \psi\frac{\omega\mu}{k_\gamma^2}\overline{\partial_{\nu,\alpha} z} - \psi\frac{\gamma}{k_\gamma^2}\overline{\partial_{\tau,\alpha} w} + \varphi\frac{\gamma}{k_\gamma^2}\overline{\partial_{\tau,\alpha} z}\right) = 0\,,\end{aligned}$$

hence the solution (w,z) of the adjoint problem (4.4) satisfies the differential equations

$$(\Delta_\alpha + \overline{k_\gamma^2})\, w = (\Delta_\alpha + \overline{k_\gamma^2})\, z = 0 \quad \text{in } \Omega \tag{4.5}$$

together with the transmission conditions

$$\begin{gathered}[w]_\Lambda = [z]_\Lambda = 0\\ \left[\frac{\gamma}{\overline{k_\gamma^2}}\partial_{\tau,\alpha} w - \frac{\omega\mu}{\overline{k_\gamma^2}}\partial_{\nu,\alpha} z\right]_{\Lambda_j} = \left[\frac{\gamma}{\overline{k_\gamma^2}}\partial_{\tau,\alpha} z + \frac{\omega\overline{\epsilon}}{\overline{k_\gamma^2}}\partial_{\nu,\alpha} w\right]_\Lambda = 0\,.\end{gathered} \tag{4.6}$$

Now, from (4.3) and (4.4) we see that

$$DF(\chi) = \mathcal{B}\left(\binom{u_1}{v_1},\binom{w}{z}\right),$$

which together with Theorem 3.2 proves the following

THEOREM 4.1 The derivative of the cost function F with respect to the variation (3.3) of the interface Λ is given by the formula

$$DF(\chi) = -B_{\epsilon,1}(u,w) - B_{\mu,1}(v,z) + C_1(v,w) - C_1(u,z)\,, \tag{4.7}$$

where the sesquilinear forms $B_{\epsilon,1}$, $B_{\mu,1}$ and C_1 are defined by (3.5), (3.6), and (u,v) and (w,z) denote the solutions of the direct and adjoint diffraction problems (2.20), (4.4), respectively.

5. Derivatives of grating efficiencies as interface integrals

Theorem 4.1 states that the derivative of the cost functional can be obtained from certain integrals with supp $\nabla\chi$ as domain of integration. In the following formula (4.7) will be simplified by transforming these domain integrals to contour integrals. In this section we will only consider the variation of interfaces between two different materials. This means the support of the function χ is divided by some part of the interface Λ into two subdomains Ω^+ and Ω^- where the functions ϵ, k take constant values, denoted by ϵ_+, k_+ and ϵ_-, k_-, respectively.

Let $\Gamma \subset \Omega$ be a simple closed piecewise smooth curve enclosing the domain G such that $\epsilon = const$ in G. Let $\nu = (\nu_1,\nu_2)$ be the exterior normal to Γ. We denote by $B_{\epsilon,1}(u,w;G)$, $C_1(u,z;G)$ the forms (3.5) and (3.6), respectively, where the integrals are taken over G instead of Ω.

LEMMA 5.1 ([11]) If u, w solve the Helmholtz equations

$$(\Delta_\alpha + k_\gamma^2)\, u = (\Delta_\alpha + \overline{k_\gamma^2})\, w = 0 \quad \text{in} \quad G \tag{5.1}$$

and $\operatorname{supp}\chi \cap \Gamma$ does not contain a corner point of Λ, then

$$B_{\epsilon,1}(u, w; G) = \int_\Gamma \frac{\omega\epsilon}{k_\gamma^2}\Big((\chi,\nu)\mathcal{J}(u,w) + (\chi,\tau)\mathcal{K}(u,w) + \chi_1\mathcal{L}(u,w)\Big)\,, \tag{5.2}$$

where

$$\begin{aligned}
\mathcal{J}(u,w) &= (\partial_{\tau,\alpha} u\, \overline{\partial_{\tau,\alpha} w} - \partial_{\nu,\alpha} u\, \overline{\partial_{\nu,\alpha} w}) - k_\gamma^2 u\overline{w} \qquad (5.3)\\
\mathcal{K}(u,w) &= -(\partial_{\nu,\alpha} u\, \overline{\partial_{\tau,\alpha} w} + \partial_{\tau,\alpha} u\, \overline{\partial_{\nu,\alpha} w})\,,\ \mathcal{L}(u,w) = i\alpha(u\, \overline{\partial_{\nu,\alpha} w} - \partial_{\nu,\alpha} u\, \overline{w})\,.
\end{aligned}$$

The proof follows from repeated application of Green's formula to (3.5), which is justified since $u, w \in H^2(\operatorname{supp}\chi \cap G)$.

REMARK 5.1 If $\epsilon = const$ and $\chi = const$ in G and ∂G does not contain singular points of the interface Λ, then from (3.5) and Lemma 5.1 it is clear that

$$\int_{\partial G} \Big((\chi,\nu)\mathcal{J}(u,w) + (\chi,\tau)\mathcal{K}(u,w) + \chi_1\mathcal{L}(u,w)\Big) = 0$$

for any function u, w satisfying the equations (5.1). Moreover, by Green's formula we have

$$\int_{\partial G} \mathcal{L}(u,w) = i\alpha \int_{\partial G} (u\, \overline{\partial_{\nu,\alpha} w} - \partial_{\nu,\alpha} u\, \overline{w}) = 0\,,$$

implying

$$\int_{\partial G} \frac{\omega\epsilon}{k_\gamma^2}\Big((\chi,\nu)\mathcal{J}(u,w) + (\chi,\tau)\mathcal{K}(u,w)\Big) = 0\,.$$

Green's formula applied to the domain integrals in (3.6) leads to

LEMMA 5.2 For any $\varphi, \psi \in H^1(G)$

$$C_1(\varphi,\psi;G) = \int_\Gamma \frac{i\alpha\gamma}{k_\gamma^2}\chi_1(\nu_1\partial_2(\varphi\overline{\psi}) - \nu_2\partial_1(\varphi\overline{\psi})) = \int_\Gamma \frac{i\alpha\gamma}{k_\gamma^2}\chi_1(\partial_{\tau,\alpha}\varphi\,\overline{\psi} + \varphi\,\overline{\partial_{\tau,\alpha}\psi})\,. \tag{5.4}$$

The following corollary contains, in particular, our final result in the case of smooth interfaces.

COROLLARY 5.1 If Λ has no corner points in $\operatorname{supp}\chi$, then

$$DF(\chi) = -\int_\Lambda (\chi,\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w) + \frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big]_\Lambda\,. \tag{5.5}$$

Here ν denotes the normal to Λ pointing from Ω^+ into Ω^- and $[v]_\Lambda$ stands for the jump $v|_\Lambda^+ - v|_\Lambda^-$ across Λ, where $v|_\Lambda^\pm$ represents the limit as the interface is approached from the region $\Omega^\pm$.

Proof. Applying Lemma 5.1 with $G = \Omega^{\pm}$, we obtain

$$
\begin{aligned}
&B_{\epsilon,1}(u,w) = B_{\epsilon,1}(u,w;\Omega^+) + B_{\epsilon,1}(u,w;\Omega^-) \\
&= \int_{\Lambda} \frac{\omega\epsilon_+}{k_\gamma^2}\Big((\chi,\nu)\mathcal{J}|_{\Lambda}^{+} + (\chi,\tau)\mathcal{K}|_{\Lambda}^{+} + \chi_1\mathcal{L}|_{\Lambda}^{+}\Big) - \int_{\Lambda} \frac{\omega\epsilon_-}{k_\gamma^2}\Big((\chi,\nu)\mathcal{J}|_{\Lambda}^{-} + (\chi,\tau)\mathcal{K}|_{\Lambda}^{-} + \chi_1\mathcal{L}|_{\Lambda}^{-}\Big) \\
&= \int_{\Lambda} (\chi,\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)\Big]_{\Lambda} + \int_{\Lambda} (\chi,\tau)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{K}(u,w)\Big]_{\Lambda} + \int_{\Lambda} \chi_1\Big[\frac{i\alpha\omega\epsilon}{k_\gamma^2}(u\,\overline{\partial_{\nu,\alpha}w} - \partial_{\nu,\alpha}u\,\overline{w})\Big]_{\Lambda}
\end{aligned}
$$

and

$$
\begin{aligned}
&B_{\mu,1}(v,z) = B_{\mu,1}(v,z;\Omega^+) + B_{\mu,1}(v,z;\Omega^-) \\
&= \int_{\Lambda} (\chi,\nu)\Big[\frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big]_{\Lambda} + \int_{\Lambda} (\chi,\tau)\Big[\frac{\omega\mu}{k_\gamma^2}\mathcal{K}(v,z)\Big]_{\Lambda} + \int_{\Lambda} \chi_1\Big[\frac{i\alpha\omega\mu}{k_\gamma^2}(v\,\overline{\partial_{\nu,\alpha}z} - \partial_{\nu,\alpha}v\,\overline{z})\Big]_{\Lambda}.
\end{aligned}
$$

From Lemma 5.2 one has

$$
\begin{aligned}
&C_1(v,w) - C_1(u,z) = C_1(v,w;\Omega^+) + C_1(v,w;\Omega^-) - C_1(u,z;\Omega^+) - C_1(u,z;\Omega^-) \\
&= \int_{\Gamma} \chi_1\Big[\frac{i\alpha\gamma}{k_\gamma^2}(\partial_{\tau,\alpha}v\,\overline{w} + v\,\overline{\partial_{\tau,\alpha}w})\Big]_{\Lambda} - \int_{\Gamma} \chi_1\Big[\frac{i\alpha\gamma}{k_\gamma^2}(\partial_{\tau,\alpha}u\,\overline{z} + u\,\overline{\partial_{\tau,\alpha}z})\Big]_{\Lambda}.
\end{aligned}
$$

Collecting in $DF(\chi) = -B_{\epsilon,1}(u,w) - B_{\mu,1}(v,z) + C_1(v,w) - C_1(u,z)$ the terms containing the factor $i\alpha$ then gives

$$
\begin{aligned}
&i\alpha\int_{\Gamma} \chi_1\Big[\frac{\gamma}{k_\gamma^2}(\partial_{\tau,\alpha}v\,\overline{w} + v\,\overline{\partial_{\tau,\alpha}w} - \partial_{\tau,\alpha}u\,\overline{z} - u\,\overline{\partial_{\tau,\alpha}z})\Big]_{\Lambda} \\
&-i\alpha\int_{\Gamma} \chi_1\Big[\frac{\omega\epsilon}{k_\gamma^2}(u\,\overline{\partial_{\nu,\alpha}w} - \partial_{\nu,\alpha}u\,\overline{w}) + \frac{\omega\mu}{k_\gamma^2}(v\,\overline{\partial_{\nu,\alpha}z} - \partial_{\nu,\alpha}v\,\overline{z})\Big]_{\Lambda} \\
&= i\alpha\int_{\Gamma} \chi_1\left(\Big[\frac{\gamma}{k_\gamma^2}\partial_{\tau,\alpha}v + \frac{\omega\epsilon}{k_\gamma^2}\partial_{\nu,\alpha}u\Big]_{\Lambda}\overline{w} - \Big[\frac{\gamma}{k_\gamma^2}\partial_{\tau,\alpha}u - \frac{\omega\mu}{k_\gamma^2}\partial_{\nu,\alpha}v\Big]_{\Lambda}\overline{z}\right) \\
&+i\alpha\int_{\Gamma} \chi_1\left(v\Big[\frac{\gamma}{k_\gamma^2}\overline{\partial_{\tau,\alpha}w} - \frac{\omega\mu}{k_\gamma^2}\overline{\partial_{\nu,\alpha}z}\Big]_{\Lambda} - u\Big[\frac{\gamma}{k_\gamma^2}\overline{\partial_{\tau,\alpha}z} + \frac{\omega\epsilon}{k_\gamma^2}\overline{\partial_{\nu,\alpha}w}\Big]_{\Lambda}\right) = 0
\end{aligned}
$$

due to the transmission conditions (2.10) and (4.6) for the solutions (u,v) and (w,z). The same relations also imply

$$
\begin{aligned}
&\int_{\Lambda} (\chi,\tau)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{K}(u,w)\Big]_{\Lambda} + \int_{\Lambda} (\chi,\tau)\Big[\frac{\omega\mu}{k_\gamma^2}\mathcal{K}(v,z)\Big]_{\Lambda} \\
&= \int_{\Lambda} (\chi,\tau)\left(\Big[\frac{\gamma}{k_\gamma^2}(\partial_{\tau,\alpha}v\,\overline{\partial_{\tau,\alpha}w} + \partial_{\tau,\alpha}u\,\overline{\partial_{\tau,\alpha}z})\Big]_{\Lambda} - \Big[\frac{\gamma}{k_\gamma^2}(\partial_{\tau,\alpha}u\,\overline{\partial_{\tau,\alpha}z} + \partial_{\tau,\alpha}v\,\overline{\partial_{\tau,\alpha}w})\Big]_{\Lambda}\right) = 0.
\end{aligned}
$$

∎

REMARK 5.2 Since μ is constant and v, z are continuous across Λ, we have

$$
\Big[\frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big]_{\Lambda} = \Big[\frac{\omega\mu}{k_\gamma^2}(\partial_{\tau,\alpha}v\,\overline{\partial_{\tau,\alpha}z} - \partial_{\nu,\alpha}v\,\overline{\partial_{\nu,\alpha}z})\Big]_{\Lambda},
$$

whereas

$$
\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)\Big]_{\Lambda} = \Big[\frac{\omega\epsilon}{k_\gamma^2}(\partial_{\tau,\alpha}u\,\overline{\partial_{\tau,\alpha}w} - \partial_{\nu,\alpha}u\,\overline{\partial_{\nu,\alpha}w}) - \omega\epsilon\,u\overline{w}\Big]_{\Lambda}.
$$

We now extend formula (5.5) to the case that supp χ contains corner points of Λ. It is well known that non–smooth boundaries or interfaces give rise to corner singularities of solutions to partial differential equations. For the conical diffraction problem (2.20), these corner singularities were studied in [12]. Assume that Λ has exactly one corner point at O, and denote by δ the angle at O seen from Ω^+. Without loss of generality we may assume that Ω^+ locally coincides with the sector $\{(r,\varphi) : 0 < r < \infty, |\varphi| < \delta/2\}$, where (r,φ) denote polar coordinates centered at O. Then the solution $(u,v) \in (H^1_p(\Omega))^2$ satisfies

$$\xi u|_{\Omega^\pm} = C_u + C\, r^{\lambda_0}\, u_0^\pm + u_1\,, \quad \xi v|_{\Omega^\pm} = C_v + C\, r^{\lambda_0}\, v_0^\pm + v_1\,, \tag{5.6}$$

where C_u, C_v and C are certain constants, ξ is a smooth cut–off function near O, the remainder terms u_1, v_1 satisfy

$$u_1|_{\Omega^\pm}, v_1|_{\Omega^\pm} \in H^{2-\varepsilon}(\Omega^\pm) \quad \text{for all} \quad \varepsilon > 0\,,$$

and λ_0 is the unique zero of the transcendental equation

$$\frac{\sin(\pi-\delta)\lambda}{\sin\pi\lambda} = \rho\,\frac{\epsilon_- + \epsilon_+}{\epsilon_- - \epsilon_+}\,, \qquad \rho = \pm 1 \tag{5.7}$$

in the strip $0 < \operatorname{Re}\lambda < 1$, which exists if $|\epsilon_+/\epsilon_-| \neq 1$. Moreover, the functions $u_0^\pm, v_0^\pm$ take the form

$$\begin{aligned} (u_0^+, v_0^+) &= \Big(\frac{\gamma}{\omega\epsilon_+}\cos\lambda(\pi-\frac{\delta}{2})\,\sin\lambda\phi\,,\ \cos\lambda(\pi-\frac{\delta}{2})\,\cos\lambda\phi\Big)\,, \quad \phi\in(-\frac{\delta}{2},\frac{\delta}{2})\,,\\ (u_0^-, v_0^-) &= \Big(\frac{\gamma}{\omega\epsilon_-}\cos\frac{\lambda\delta}{2}\,\sin\lambda(\phi-\pi)\,,\ \cos\frac{\lambda\delta}{2}\,\cos\lambda(\phi-\pi)\Big)\,, \quad \phi\in(\frac{\delta}{2},2\pi-\frac{\delta}{2})\,, \end{aligned} \tag{5.8}$$

if λ_0 solves (5.7) with $\rho = 1$. Note that $\gamma = \omega\sqrt{\mu\epsilon^+}\sin\phi$, where ϵ^+ denotes the dielectric coefficient of the medium above the grating. If λ_0 solves (5.7) with $\rho = -1$, then

$$\begin{aligned} (u_0^+, v_0^+) &= \Big(\frac{\gamma}{\omega\epsilon_+}\sin\lambda(\frac{\delta}{2}-\pi)\,\cos\lambda\phi\,,\ \sin\lambda(\pi-\frac{\delta}{2})\,\sin\lambda\phi\Big)\,, \quad \phi\in(-\frac{\delta}{2},\frac{\delta}{2})\,,\\ (u_0^-, v_0^-) &= \Big(\frac{\gamma}{\omega\epsilon_-}\sin\frac{\lambda\delta}{2}\,\cos\lambda(\phi-\pi)\,,\ \sin\frac{\lambda\delta}{2}\,\sin\lambda(\pi-\phi)\Big)\,, \quad \phi\in(\frac{\delta}{2},2\pi-\frac{\delta}{2})\,. \end{aligned} \tag{5.9}$$

It is clear from (4.5), (4.6) that the complex conjugate $(\overline{w},\overline{z})$ of the solution of the adjoint problem (4.4) also admits the representation (5.6) with other constants C, C_w, C_z and remainder terms. Hence, if $\operatorname{Re}\lambda_0 > 1/2$ then the solutions (u,v) and (w,z) belong to $H^{3/2+\varepsilon}(\Omega^\pm)$ for some $\varepsilon > 0$, ensuring that the line integrals in the gradient formula (5.5) exist. Note that the condition $\operatorname{Re}\lambda_0 > 1/2$ is always satisfied if $\epsilon_\pm$ are real; see [6]. If three materials with real dielectric constants ϵ meet at some corner points then this condition holds if the maximum angle is less or equal π. This follows from a recent result of Petzoldt [16].

Formula (5.5) has to be modified if strong corner singularities (with $\operatorname{Re}\lambda_0 < 1/2$) occur. For TM diffraction problems, this was done in [11, Theorem 4.4] where the explicit knowledge of the functions $v_0^\pm$ was employed to express the limit

$$\lim_{\varepsilon\to 0}\Big(B_{1,\mu}(v,z;\Omega_\varepsilon^+) + B_{1,\mu}(v,z;\Omega_\varepsilon^-)\Big) = B_{1,\mu}(v,z)$$

as a contour integral plus some remainder term, where $\Omega_\varepsilon^\pm = \Omega^\pm \setminus \{r \leqslant \varepsilon\}$. Since for conical diffraction the coefficient functions $u_0^\pm, v_0^\pm$ are the same as for the TM problem, one can show by repeating the arguments of [11] that

$$\lim_{\varepsilon\to 0} \Big(B_{1,\epsilon}(u,w;\Omega_\varepsilon^+) + B_{1,\epsilon}(u,w;\Omega_\varepsilon^-) \Big)$$
$$= \lim_{\varepsilon\to 0} \Big(\frac{\varepsilon}{2\lambda_0 - 1} (\mathcal{G}(O_{-\varepsilon}) + \mathcal{G}(O_\varepsilon)) + \int_{\Lambda_\varepsilon} \mathcal{G} \Big) + \int_\Lambda \chi_1 \Big[\frac{i\alpha\omega\epsilon}{k_\gamma^2} (u\, \overline{\partial_{\nu,\alpha} w} - \partial_{\nu,\alpha} u\, \overline{w}) \Big]_\Lambda .$$

Here we used the notation $\mathcal{G} := \Big[\frac{\omega\epsilon}{k_\gamma^2} ((\chi,\nu)\mathcal{J}(u,w) + (\chi,\tau)\mathcal{K}(u,w)) \Big]_\Lambda$, $\Lambda_\varepsilon = \Lambda \setminus (\overline{OO_{-\varepsilon}} \cup \overline{OO_\varepsilon})$, where the two points $O_{\pm\varepsilon}$ on Λ satisfy $\operatorname{dist}(O, O_{\pm\varepsilon}) = \varepsilon$.

Analogously, for the form $B_{1,\mu}(v,z)$ we have

$$B_{1,\mu}(v,z) = \lim_{\varepsilon\to 0} \Big(\frac{\varepsilon}{2\lambda_0 - 1} (\mathcal{H}(O_{-\varepsilon}) + \mathcal{H}(O_\varepsilon)) + \int_{\Lambda_\varepsilon} \mathcal{H} \Big) + \int_\Lambda \chi_1 \Big[\frac{i\alpha\omega\mu}{k_\gamma^2} (v\, \overline{\partial_{\nu,\alpha} z} - \partial_{\nu,\alpha} u\, \overline{w}) \Big]_\Lambda$$

with $\mathcal{H} := \Big[\frac{\omega\mu}{k_\gamma^2} ((\chi,\nu)\mathcal{J}(v,z) + (\chi,\tau)\mathcal{K}(v,z)) \Big]_\Lambda$. Using the transmission conditions as in the proof of Corollary 5.1, one obtains

THEOREM 5.1 If $\Lambda \cap$ supp χ contains exactly one corner point at O, then

$$DF(\chi) = \lim_{\varepsilon\to 0} \Big(\frac{\varepsilon}{2\lambda_0 - 1} (\mathcal{Y}(O_{-\varepsilon}) + \mathcal{Y}(O_\varepsilon)) + \int_{\Lambda_\varepsilon} \mathcal{Y} \Big), \tag{5.10}$$

where

$$\mathcal{Y} = (\chi,\nu) \Big[\frac{\omega\epsilon}{k_\gamma^2} \mathcal{J}(u,w) + \frac{\omega\mu}{k_\gamma^2} \mathcal{J}(v,z) \Big]_\Lambda$$

and the form $\mathcal{J}$ is defined in (5.3).

REMARK 5.3 Since $\mathcal{Y}(x) = O(r^{2\lambda_0 - 2})$ as $r \to 0$, the formula (5.10) coincides with formula (5.5) if Re $\lambda_0 > 1/2$.

REMARK 5.4 The extension of (5.10) to the case of finitely many corners $O_1, \ldots, O_r$ of Λ with angles $\delta_1, \ldots, \delta_r$ is straightforward. Introducing the points $O_{j,\pm\varepsilon} \in \Lambda$ with $\operatorname{dist}(O_j, O_{j,\pm\varepsilon}) = \varepsilon$, formula (5.10) then holds with $\Lambda_\varepsilon = \Lambda \setminus \bigcup_{j=1}^r (\overline{O_j O_{j,-\varepsilon}} \cup \overline{O_j O_{j,\varepsilon}})$ and the correction terms replaced by the sum

$$\sum_{j=1}^r \frac{\varepsilon}{2\lambda_j - 1} (\mathcal{Y}(O_{j,-\varepsilon}) + \mathcal{Y}(O_{j,\varepsilon})) \Big),$$

where λ_j denotes the root of equation (5.7) (with $\delta = \delta_j$) in the strip $0 < \operatorname{Re}\lambda < 1$.

6. Derivatives of grating efficiencies as contour integrals

Formula (5.10) requires the knowledge of the zero λ_0 of the transcendental equation (5.7). An alternative representation of $DF(\chi)$ can be given by a path–independent contour integral; see Theorem 6.1 below. In contrast to Theorem 5.1, the result is also valid if several materials meet at some interior point O with angles different from zero. Under this assumption, it is known [13] that the solutions of the direct problem belong to $H_p^{1+\varepsilon}(\Omega)$ for some $\varepsilon > 0$ and admit the asymptotics

$$\xi u = C_u + C\, r^{\lambda_0} p_\ell(\log r)\, u_0 + u_1 \,, \tag{6.1}$$

with $\operatorname{Re}\lambda_0 > \varepsilon$. Here p_ℓ is some polynomial of degree ℓ, the 2π–periodic function $u_0 = u_0(\phi)$ is continuous and $u_1 \in H_p^{1+\delta}(\Omega)$, $\delta > \varepsilon$. A generalization of Theorem 5.1 to the case of interface intersection points would require more detailed information about the second term on the right–hand side of (6.1), which presently seems to be not available.

We first extend formula (5.2) and the corresponding representation of the form $B_{\mu,1}$ to the case where $\operatorname{supp}\chi$ contains a singular interface point. Recall that Ω_j, $j = 1, \dots, m$, are the subdomains of Ω where $\epsilon = const.$

Lemma 6.1 Suppose that $\operatorname{supp}\chi$ contains exactly one corner or intersection point O of Λ. Then for any Ω_j

$$\begin{aligned}
B_{\epsilon,1}(u,w;\Omega_j) &= \int\limits_{\partial\Omega_j} \frac{\omega\epsilon}{k_\gamma^2}\Big((\chi-\chi(O),\nu)\mathcal{J}(u,w) + (\chi-\chi(O),\tau)\mathcal{K}(u,w) + \chi_1\mathcal{L}(u,w)\Big)\,,\\
B_{\mu,1}(v,z;\Omega_j) &= \int\limits_{\partial\Omega_j} \frac{\omega\mu}{k_\gamma^2}\Big((\chi-\chi(O),\nu)\mathcal{J}(v,z) + (\chi-\chi(O),\tau)\mathcal{K}(v,z) + \chi_1\mathcal{L}(v,z)\Big)\,,
\end{aligned}$$

where (u,v) and (w,z) solve the direct and adjoint problems (2.20), (4.4), respectively.

Proof. Suppose that O is a boundary point of $G = \Omega_j$, and let $G_\varepsilon = G \setminus \{r \leqslant \varepsilon\}$, $r = \operatorname{dist}(x, O)$. Consider the form $B_{\epsilon,1}$, for example. From Remark 5.1 we have

$$\int\limits_{\partial G_\varepsilon} \frac{\omega\epsilon}{k_\gamma^2}\Big((\chi(O),\nu)\mathcal{J}(u,w) + (\chi(O),\tau)\mathcal{K}(u,w)\Big) = 0\,.$$

Hence, from Lemma 5.1

$$B_{\epsilon,1}(u,w;G_\varepsilon) = \int\limits_{\partial G_\varepsilon} \frac{\omega\epsilon}{k_\gamma^2}\Big((\chi-\chi(O),\nu)\mathcal{J}(u,w) + (\chi-\chi(O),\tau)\mathcal{K}(u,w) + \chi_1\mathcal{L}(u,w)\Big)\,,$$

and using the asymptotics of u and $\overline{w}$ one can pass to the limit. ∎

Theorem 6.1 Assume that Λ contains exactly one corner or intersection point O, and let $\Gamma = \partial G \subset \Omega$ be an arbitrary simple closed piecewise smooth curve around that point.

Then, with the sesquilinear forms $\mathcal{J}$ and $\mathcal{K}$ defined in (5.3), we have

$$\begin{aligned} DF(\chi) = & \int_{\Gamma} (\chi(O),\nu)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w) + \frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big) \\ & + \int_{\Gamma} (\chi(O),\tau)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{K}(u,w) + \frac{\omega\mu}{k_\gamma^2}\mathcal{K}(v,z)\Big) \\ & - \int_{G\cap\Lambda} (\chi-\chi(O),\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w) + \frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big]_{\Lambda} \\ & - \int_{\Lambda\setminus G} (\chi,\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w) + \frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big]_{\Lambda}. \end{aligned} \tag{6.2}$$

Proof. Applying Lemma 6.1 to the subdomains Ω_j and summing over j gives

$$\begin{aligned} B_{\epsilon,1}(u,w) = & \sum_{j=1}^{m} B_{\epsilon,1}(u,w;\Omega_j) \\ = & \int_{\partial\Omega} \frac{\omega\epsilon}{k_\gamma^2}\Big((\chi-\chi(O),\nu)\mathcal{J}(u,w) + (\chi-\chi(O),\tau)\mathcal{K}(u,w) + \chi_1\mathcal{L}(u,w)\Big) \\ & + \int_{\Lambda}\Big((\chi-\chi(O),\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)\Big]_{\Lambda} + (\chi-\chi(O),\tau)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{K}(u,w)\Big]_{\Lambda} + \chi_1\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{L}(u,w)\Big]_{\Lambda}\Big) \\ = & -\int_{\partial\Omega} \frac{\omega\epsilon}{k_\gamma^2}\Big((\chi(O),\nu)\mathcal{J}(u,w) + (\chi(O),\tau)\mathcal{K}(u,w)\Big) \\ & + \int_{\Lambda}\Big((\chi-\chi(O),\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)\Big]_{\Lambda} + (\chi-\chi(O),\tau)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{K}(u,w)\Big]_{\Lambda} + \chi_1\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{L}(u,w)\Big]_{\Lambda}\Big). \end{aligned}$$

Similarly to the proof of Corollary 5.1, we obtain by using the transmission conditions for (u,v) and (w,z) on Λ

$$\begin{aligned} & B_{\epsilon,1}(u,w) + B_{\mu,1}(v,z) - C_1(v,w) + C_1(u,z) \\ & = -\int_{\partial\Omega}\Big((\chi(O),\nu)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w) + \frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big) + (\chi(O),\tau)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{K}(u,w) + \frac{\omega\mu}{k_\gamma^2}\mathcal{K}(v,z)\Big)\Big) \\ & \quad + \int_{\Lambda}(\chi-\chi(O),\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w) + \frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big]_{\Lambda}, \end{aligned}$$

which proves (6.2) for $\Gamma = \partial\Omega$. Furthermore, Remark 5.1 applied to the subdomains $\Omega_j \setminus G$ gives

$$\int_{\partial(\Omega_j\setminus G)} \Big((\chi(O),\nu)\mathcal{J}(u,w) + (\chi(O),\tau)\mathcal{K}(u,w)\Big) = 0\,,$$

hence, again by using the transmission conditions for (u,v) and (w,z) one obtains

$$\int_{\partial\Omega}\Big((\chi(O),\nu)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)+\frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big)+(\chi(O),\tau)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{K}(u,w)+\frac{\omega\mu}{k_\gamma^2}\mathcal{K}(v,z)\Big)\Big)$$
$$=\int_{\Gamma}\Big((\chi(O),\nu)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)+\frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big)+(\chi(O),\tau)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{K}(u,w)+\frac{\omega\mu}{k_\gamma^2}\mathcal{K}(v,z)\Big)\Big)$$
$$-\int_{\Lambda\setminus G}(\chi(O),\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)+\frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big]_\Lambda.\ \blacksquare$$

REMARK 6.1 Formula (6.2) easily extends to the case of finitely many singular points $O_1,\dots,O_r$ of the interface Λ. Let $\Gamma_j=\partial G_j$ be a simple piecewise smooth curve enclosing the singular point O_j only. Then the right–hand side of (6.2) has to be replaced by the sum

$$\begin{aligned}\sum_j\Big(&\int_{\Gamma_j}(\chi(O_j),\nu)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)+\frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big)\\&+\int_{\Gamma_j}(\chi(O_j),\tau)\Big(\frac{\omega\epsilon}{k_\gamma^2}\mathcal{K}(u,w)+\frac{\omega\mu}{k_\gamma^2}\mathcal{K}(v,z)\Big)\\&-\int_{G_j\cap\Lambda}(\chi-\chi(O_j),\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)+\frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big]_\Lambda\Big)\\&-\int_{\Lambda\setminus(\cup G_j)}(\chi,\nu)\Big[\frac{\omega\epsilon}{k_\gamma^2}\mathcal{J}(u,w)+\frac{\omega\mu}{k_\gamma^2}\mathcal{J}(v,z)\Big]_\Lambda.\end{aligned}\qquad(6.3)$$

7. An application to coated gratings

Finally we apply the gradient formula to a simple example. A periodic binary structure is etched into a substrate material and a coating is deposit as shown in Figure 1.

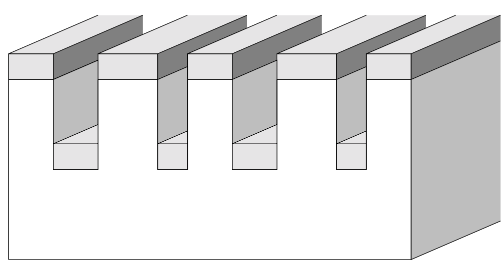

FIG. 1. Coated binary grating

We are interested in the derivative of the cost functional F with respect to variations of the grating depth t with fixed thickness c of the coating.

The corresponding computational domain Ω is shown in Figure 2. The variation of the grating depth t can be given by the function $\chi=(0,\chi_2(x_2))$, where χ_2 is compactly supported in $[t-\delta,t+c+\delta]$ with $\chi_2(x_2)=1$, $t\leqslant x_2\leqslant t+c$.

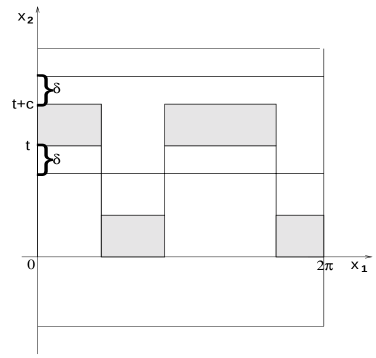

FIG. 2. Computational domain for the coated binary grating

Thus the support of χ contains several singular points O_j. However, since $\chi(O_j) = (0,1)$ for all of those points, one can apply Theorem 6.1 directly. If $G = [0, 2\pi] \times [t-\delta, t+c+\delta]$ then on $\Lambda \setminus G$ we have $\chi = 0$. Moreover, for the horizontal pieces of $G \cap \Lambda$ one has $\chi = (0,1)$, whereas $(\chi - (0,1), \nu) = 0$ for the vertical pieces. Therefore in formula (6.2) only the integral over the two lines $S_1 = \{t+c+\delta\} \times [0, 2\pi]$ and $S_2 = \{t-\delta\} \times [0, 2\pi]$ (the boundary of G) remain, and the gradient can be computed from

$$DF(\chi) = \int\limits_{S_1} \Big(\frac{\omega\epsilon}{k_\gamma^2} (\partial_{1,\alpha} u \, \overline{\partial_{1,\alpha} w} - \partial_2 u \, \overline{\partial_2 w}) - \omega\epsilon u \overline{w} + \frac{\omega\mu}{k_\gamma^2} (\partial_{1,\alpha} v \, \overline{\partial_{1,\alpha} z} - \partial_2 v \, \overline{\partial_2 z}) - \omega\mu v \overline{z} \Big)$$
$$- \int\limits_{S_2} \Big(\frac{\omega\epsilon}{k_\gamma^2} (\partial_{1,\alpha} u \, \overline{\partial_{1,\alpha} w} - \partial_2 u \, \overline{\partial_2 w}) - \omega\epsilon u \overline{w} + \frac{\omega\mu}{k_\gamma^2} (\partial_{1,\alpha} v \, \overline{\partial_{1,\alpha} z} - \partial_2 v \, \overline{\partial_2 z}) - \omega\mu v \overline{z} \Big).$$

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